QUALITY OF SYNTHETIC GASOLINE FROM COAL

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Introduction

Gasoline can be produced from coal by a two stage process wherein coal gets converted to a synthetic crude by hydrogenation, solvent extraction, pyrolysis or carbonization in the first stage and the synthetic crude thus produced gets converted to gasoline in the second stage by hydroprocessing. The quality of gasoline depends upon the type of coal, the coal conversion process, the quality of the synthetic crude and the conditions of hydroprocessing of the crude. Coal gasolines are expected to be high in aromatic content (60-90%) when compared to petroleum gasolines since they are produced from highly aromatic (>75% aromatics) feed stocks. They, therefore, will have high octane ratings. Air quality standards may forbid the use of such high aromatic gasolines in automobiles in the very near future and it, therefore, becomes necessary to reduce the aromaticity of coal gasoline to make it acceptable. Though the coal derived gasolines are known to be high in aromatic content and octane value, not much data was published in the literature on their nature and quality. Qader and Hill[1] reported the preparation of coal naphthas by the hydrocracking of coal oils in a bench scale fixed bed system. High quality naphthas having very small quantities of sulfur, nitrogen and oxygen were obtained. The clear research octane numbers of the naphthas varied between 80 and 91. In the present investigation, data on the production of gasoline from different coal oils by hydroprocessing and the nature of the products are reported. Production of low aromatic gasolines from coal gasoline and its effect on the economics of the coal hydrogenation process are discussed. A case for the production of BTX from coal is presented.

Experimental

Low temperature tar, pyrolysis tar and solvent extracted coal were prepared in laboratory scale equipment from a high volatile bituminous coal from Utah[2]. Hydrogenation oil (coal oil) was prepared in a bench scale free fall dilute phase system[3] from the same coal. Commercial catalysts were used in the hydrorefining and hydrocracking of coal oils[4]. The evaluation of the raw materials and products was done by standard methods.

Gasoline was prepared from coal oil by hydrorefining and hydrocracking in a fixed bed reactor[1]. The aromatics were extracted from gasoline with dimethylformamide and sulfolane in laboratory mixed-Settler apparatus at room temperature. The research octane numbers were determined in the Standard Oil Company laboratories at Salt Lake City.

Results and Discussion

The nature of the coal oil depends upon the coal rank and the conversion process. Oils produced from the same coal and by different conversion processes will be different in nature. The data given in Table 1 shows that the composition of the coal oils is greatly influenced by the type of coal conversion process employed. The low temperature and pyrolysis tars are similar in nature except that the pyrolysis tar has slightly higher contents of sulfur, oxygen and residue while the low temperature tar has higher contents of nitrogen and asphaltenes. From a practical standpoint, they can be considered as similar in composition. The solvent extracted coal is very much different from the other coal oils. About 75% of the extract is composed of benzene insolubles and asphaltenes which make it a very inferior quality oil. It also has highest contents of sulfur, nitrogen, oxygen and residue. The oil obtained by coal hydrogenation is higher in quality when compared to other coal oils and this makes it a better feed stock for further processing.

The composition of the gasoline depends upon the nature of the coal oil. The data given in Table II show that the coal gasolines are high in aromatic content and the gasoline produced from coal hydrogenation oil has the highest aromaticity. The data given in Tables II and III also show that the different hydrocarbon types of these gasolines are similar in composition. The coal gasolines have very high octane ratings because of high aromaticities and a computation of octane numbers from Figure 2 shows that the clear research octane numbers of coal gasolines vary between 95 and 100. Though the high octane ratings of coal gasolines are desirable, the high aromaticities might pose problems in their future use in automobiles. Higher gasoline aromaticities will give rise to larger exhaust hydrocarbon emission which pollute the air. Though no limits in gasoline aromaticities are imposed at the present time, it is quite concievable that regulations to limit aromaticities will come into effect in the near future. It, therefore, becomes imperative to reduce the aromatic contents of coal gasolines when they are produced on a commercial scale. This can be accomplished in several ways and the most promising route seem to be by the separation of gasoline aromatics by solvent extraction. The aromatic extract can be dealkylated to produce either BTX or pure aromatics. In this work, gasoline aromatics were extracted and gasolines containing 30, 40 and 50 percent aromatics were prepared starting with a gasoline containing 76 percent aromatics. The clear research octane numbers of the gasolines decreased in straight line with a decrease in aromatic content as shown in Figure 2. The data show that gasoline containing about 50 percent aromatics will have a clear research octane number of about 83. The octane number can probably be improved to a rating of around 90 by properly adjusting the concentrations of individual aromatic components of the gasoline. The composition of the gasoline aromatics given in Table IV shows that 80 percent of the extract can be sold as BTX without further processing. The remaining 20 percent of the aromatics either can be used for blending the gasoline or can be converted to BTX by a mild treatment of dealkylation. The dealkylation of the aromatic extract produced BTX in a yield of about 95% as shown in Table V. The product contained about 62 percent benzene.

The separation of aromatics from the gasoline and the production of BTX affects the economics of the overall coal hydrogenation process. The data given in Table VI and Figure 3 indicate that the economics can be improved significantly by producing either gasoline and BTX or only BTX as the main products. The data also indicates that the coal to BTX route is the most economically attractive approach.

Acknowledgement

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Literature Cited

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TABLE I. PROPERTIES OF COAL OILS

	L.T. Carbonization	Pyrolysis	Solvent-Extraction	Hydrogenation
Benzene Insolubles, Wt.%	Nil	2.0	43.0	Nil
Asphaltenes, Wt.%	19.0	16.0	25.0	15.0
Light Oil (up to 200°C), Vol.%	5.0	7.0	3.0	18.0
Residual Oil, +370°C, Vol.%	27.0	30.0	50.0	25.0
Sulfur, Wt.%	0.82	0.98	1.15	0.64
Nitrogen, Wt.%	0.91	0.86	1.04	0.76
Oxygen, Wt.%	3.8	4.5	8.0	2.8
Tar Acids (200°-370°C Oil)	26.0	24.0	-	15.0
Hydrocarbon Analysis of Neutral Oil (200-370°C)				
Saturates	29.0	25.0		24.0
Olefins	15.0	17.0		11.0
Aromatics	56.0	58.0		65.0

TABLE II. COMPOSITION OF COAL GASOLINES

Temp: 480°C, Pressure: 2000 psi, Space Velocity: 1.0

Feed Stock:	L.T. Tar	Pyrolysis Tar	Hydrogenation Oil
Composition, Vol. %			
Saturates	30.0	26.0	13.0
Olefins	1.0	1.0	1.0
Aromatics	69.0	73.0	86.0

TABLE III. ANALYSIS OF GASOLINE SATURATES

Gasoline From:	L.T.Tar	Pyrolysis Tar	Hydrogenation Oil
Analysis, Vol.%			
N-Paraffins			
C_6	3.2	1.7	0.9
C_7	5.9	6.6	7.4
C_8	15.2	14.1	12.7
C_9	14.1	13.2	15.5
C_{10}	3.8	4.5	2.1
C_{11}	13.8	14.2	12.2
	56.0	54.3	50.8
Iso-paraffins			
C_6	3.1	1.9	2.8
C_7	11.2	8.3	10.1
C_8	10.1	12.0	16.2
C_9	9.8	13.3	10.0
	33.2	35.5	39.1
Cyclo-parrafins			
C_6	4.1	3.2	1.7
C_7	6.7	7.0	8.4
	10.8	10.2	10.1

TABLE IV: ANALYSIS OF GASOLINE AROMATICS

GASOLINE FROM:	L.T.TAR	PYROLYSIS TAR	HYDROGENATION
Analysis, Vol.%			
Benzene	33.9	30.7	40.4
Toluene	18.2	20.2	14.8
Ethylbenzene	4.5	2.8	5.5
Xylenes	25.8	27.2	19.4
Propylbenzenes	2.5	3.5	1.6
Butylbenzenes	9.0	7.0	11.3
Indanes	4.1	5.1	4.5
Unidentified	2.0	3.5	2.5

TABLE V. COMPOSITION OF THE DEALKYLATED PRODUCT

Temp: 450°C, Pressure: 1000 psi, Space Velocity: 1.0

Composition	Volume %
Benzene	62.5
Toluene	20.4
Ethylbenzene	3.0
Xylenes	9.1
Propylbenzenes	nil
Butylbenzenes	2.5
Indans	1.5
Unidentified	1.0

TABLE VI. ECONOMIC SUMMARY (COAL-GASOLINE-BTX)

Capacity: 100,000 BBL/Day Crude Oil or 46,000 TPD Coal

	Coal-Gasoline (Base Case) MM$	Coal-Gasoline (BTX: 15¢/Gal) MM$	Coal-BTX (Naphtha: 10¢/Gal) MM$
xed Capital:	418.5	440.6	440.6
orking Capital:	41.9	44.1	44.1
tal Investment	460.4	484.7	484.7
bt (65% of Total Investment):	299.2	325.1	325.1
uity (35% of Total Investment):	161.2	159.6	159.6
rect Plant Operating Cost:	134.8	136.5	137.0
venue Required:	196.0	200.8	200.8
edit for Byproducts:	53.7	142.8	87.9
oduction Cost of Product:			
oduction Cost of Gasoline:	142.3	57.2	-
oduction Cost of BTX:	-	-	112.1
Year Average Product Price:			
asoline ¢/Gallon:	11.9	9.9	-
X ¢/Gallon:	-	-	13.3

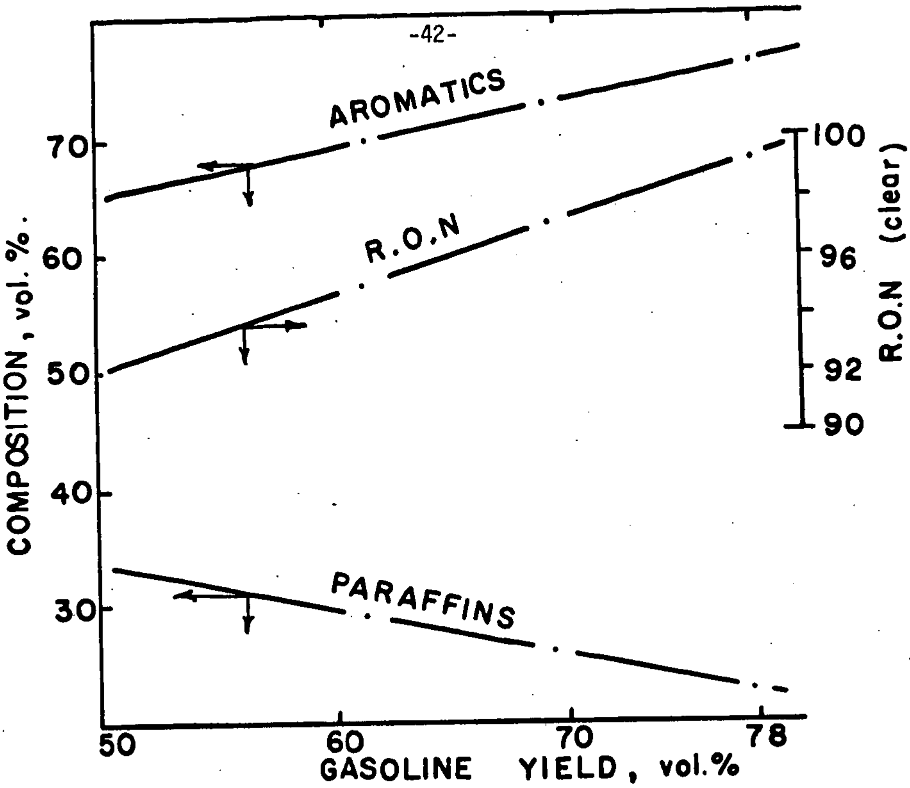

Figure I. Yield and quality of gasoline.

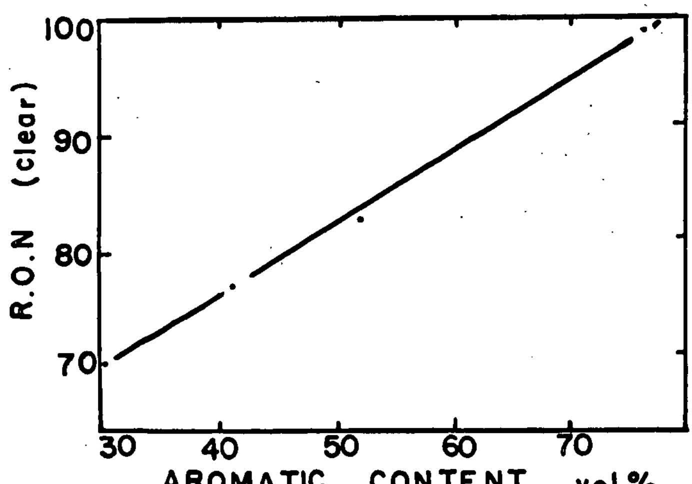

Figure 2 R.O.N and aromatic content of gasoline.

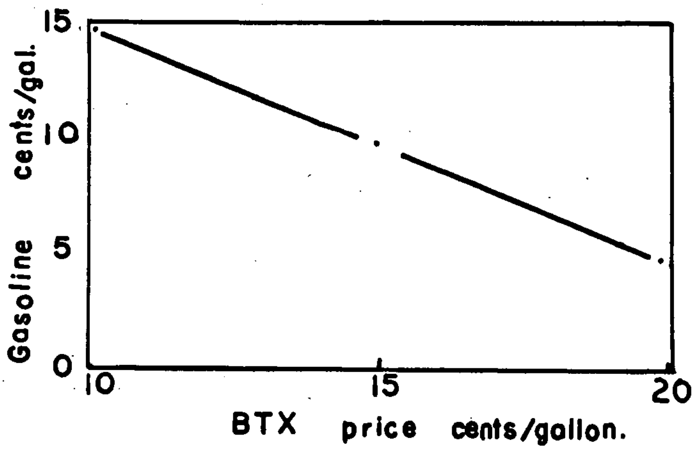

Figure 3. Variation of gasoline price with BTX price.